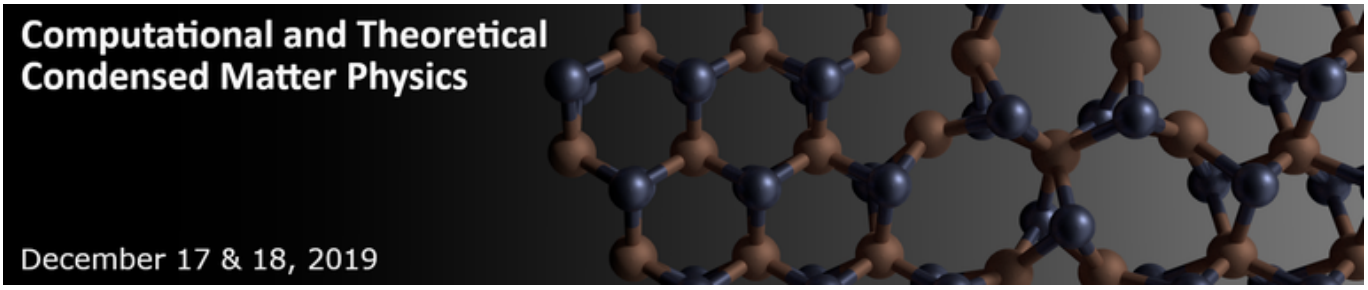

Francqui Mini-Symposium

Computational and Theoretical Condensed Matter Physics

Book of Abstracts

UNamur December 2019

Schedule

Tuesday, December 17 2019

1:00 pm		**Welcome + Introduction**	
1:20 pm	Keynote Talk 1	**Gian-Marco Rignanese**	Accelerating materials discovery through high-throughput ab initio calculations and data mining
2:00 pm	Invited Talk 1	**Jonas Bekaert**	Hydrogen-induced high-temperature superconductivity in two-dimensional materials: The example of hydrogenated monolayer MgB2
2:20 pm	Invited Talk 2	**Yoann Olivier**	Thermally Activated Delayed Fluorescence (TADF): A new paradigm for OLEDs
2:40 pm	Invited Talk 3	**Mehmet Yagmurcukardes**	Two-dimensional Ultra-thin Crystals by Chemical Conversion of van Der Waals Materials
3:00 pm	Keynote Talk 2	**Zeila Zanolli**	Spintronics at the interface
3:40 pm		**Coffee Break**	
4:20 pm	Invited Talk 4	**Nicole Helbig**	Coupled spin-lattice dynamics with multibinit
4:40 pm	Invited Talk 5	**Simon Dubois**	Understanding 2D magnetic junctions from fabrication to new functionalities
5:00 pm	Invited Talk 6	**Pedro Melo**	Spin States Protected from Intrinsic Electron−Phonon Coupling in MoSe2
5:20 pm	Invited Talk 7	**Aurelien Lherbier**	Thermal and electronic transport characteristics of highly stretchable graphene kirigami
5:40 pm	Keynote Talk 3	**Philippe Ghosez**	Origin and mechanism of the metal-insulator transition in perovskite nickelates manganites and ferrites.
6:20 pm		**Poster Session and Buffet Dinner**	

Wednesday, December 18 2019

8:30 am	Keynote Talk 4	**Ludger Wirtz**	Theoretical Spectroscopy of 2D Materials: Exciton-phonon coupling in resonant Raman and luminescence spectroscopy
9:10 am	Invited Talk 8	**Bruno Majerus**	Plasmons in nanostructured and corrugated 2D materials
9:30 am	Invited Talk 9	**Ben Van Duppen**	Graphene plasmonics: exploring the nonlocal response of 2D electron liquids
9:50 am	Invited Talk 10	**Michael Lobet**	Perfect electromagnetic absorbers: a road to reality
10:10 am		**Coffee Break**	
10:40 am	Invited Talk 11	**Tatiana Rappoport**	Two-dimensional orbital Hall insulators
11:00 am	Invited Talk 12	**Aurelie Champagne**	MXenes: the largest family of 2D materials
11:20 am	Invited Talk 13	**Thibaut Sohier**	Electron-phonon scattering in 2D materials: a quest for high conductivity
11:40 am	Invited Talk 14	**Benoit Van Troeye**	Understanding phonons in slightly-misaligned graphene bilayer with the Frenkel-Kontorova model
12:00 pm		**Wrap-up and Summary**	

Accelerating materials discovery through high-throughput ab initio calculations and data mining

Gian-Marco Rignasese

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With the progress of supercomputers and simulation codes, ab initio calculations have reached a level of maturity which makes it possible to screen thousands of materials searching for specific simple properties. In this talk, we will present this so-called high-throughput ab initio approach and the recent progress achieved in this framework. More complex properties are, however, still out of reach for this high-throughput ab initio approach. In this framework, we will present how machine learning models can be trained on a limited set of ab initio calculations to achieve interesting predictions. The potential of these two approaches will be illustrated through a few recent examples.

Hydrogen-induced high-temperature superconductivity in two-dimensional materials: The example of hydrogenated monolayer MgB_2

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In seminal work of 1968 Ashcroft predicted dense metallic hydrogen to be a high-temperature superconductor, owing to its minimal mass and resulting very high Debye temperature, enabling very strong phonon-mediated superconductivity according to the Bardeen-Cooper-Schrieffer (BCS) theory [1]. Currently, it indeed is well-established that hydrogen-based compounds under ultra-high pressure, such as the polyhydrides H3S [2] and LaH10 [3,4], superconduct through the conventional electron-phonon coupling mechanism to attain the record critical temperatures (Tc) known to date.

We will demonstrate that the intrinsic advantages of hydrogen for phonon-mediated superconductivity can be exploited in a completely different system. Namely, we found hydrogen adatoms to strongly enhance superconductivity in two-dimensional (2D) materials [5]. Firstly, Van Hove singularities in the electronic structure, originating from atomic-like hydrogen orbitals, lead to a strong increase of the electronic density of states, thus enhancing the electron-phonon coupling. Furthermore, the emergence of high-frequency hydrogen-related phonon modes in this system boosts the electron-phonon coupling further.

As a concrete example, we will focus on the effect of hydrogen adatoms on the superconducting properties of monolayer MgB2 [6,7], which we investigated by solving the fully anisotropic Eliashberg equations, in conjunction with a first-principles description of the electronic and vibrational states, and the coupling between them. We thus obtained that hydrogenation leads to an elevated Tc of 67 K, which can be boosted to over 100 K by biaxial tensile strain. This proves that hydrogenation of 2D materials can induce strong electron-phonon coupling and high-Tc superconductivity, akin to the case of the bulk hydride compounds with record Tc's [3,4], yet without the need to apply excessively high pressures that hamper practical applications.

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Thermally Activated Delayed Fluorescence (TADF): A new paradigm for OLEDs ?!?!

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Recently, Thermally Activated Delayed Fluorescence (TADF) process has appeared as the new paradigm for Organic Light-Emitting Diodes (OLEDs) allowing to beat the spin statistics limit of fluorescent emitters to reach efficiency near 100%. By design, TADF emitters have their lowest singlet and triplet excited states in near resonance so that reverse intersystem crossing (RISC) allows to upconvert the non-emissive triplets into emissive singlets. Despite all the efforts, a complete mechanistic understanding of TADF materials has not been fully uncovered yet. Part of the complexity arises from the apparent dichotomy between the need for small energy difference between the lowest singlet and triplet excited states (ΔE_{ST}) which has to carry a significant charge transfer (CT) character; and for a significant spin-orbit coupling which according to El-Sayed rules requires the involved singlet and triplet excited states to have very different natures. In this presentation, we will show:

- How the nature of these excited can be characterized and how this nature can be tuned by varying the nature of the electron donating (D) or accepting (A) units in D-A(-D) compounds.
- How this dichotomy can be resolved once accounting in a fully atomistic model of reference carbazole derivatives for thermal fluctuations of the molecular conformations and discrete electronic polarization effects in amorphous films.

For both topics, we will demonstrate that, electronic excitations involved in the TADF process have a mixed CT-locally excited character being dynamically tuned by torsional vibrational modes and that overall, the conversion of triplet-to-singlet as well as the emission is a dynamic process gated by conformational fluctuations.

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Two-Dimensional Ultra-thin Covalent Crystals by Chemical Conversion

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Most of the studied two-dimensional (2D) materials have been synthesized by exfoliation of van der Waals crystals. Recently, there has been growing interest in fabricating synthetic 2D crystals which do not have layered bulk crystal. Here, we report an approach for making 2D crystals of covalent solids by chemical conversion of van der Waals layers. As an example, we used 2D layered indium selenide (InSe) obtained by exfoliation and converted it by direct fluorination into indium fluoride (InF_3), which has a nonlayered, rhombohedral structure and therefore, cannot possibly be obtained by exfoliation. The conversion of InSe into InF_3 is found to be feasible for thicknesses down to three layers of InSe, and the obtained stable InF_3 layers are doped with selenium. The optical, electron transport, and Raman measurements of the new 2D covalent crystal are done and we show that it is a semiconductor with a direct bandgap of 2.2 eV, exhibiting high optical transparency across the visible and infrared spectral ranges. We also demonstrate the scalability of our approach by chemical conversion of large-area, thin InSe laminates obtained by liquid exfoliation, into InF3 films. The concept of chemical conversion of cleavable thin van der Waals crystals into covalently bonded noncleavable ones opens exciting prospects for synthesizing a wide variety of novel atomically thin covalent crystals.

Spintronics at the interface

Zeila Zanolli

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The interface between materials can be considered as the ultimate spintronics device, not only in terms of miniaturization but also to unlock unique design possibilities and new physical properties which are unattainable in the individual bulk materials. As device dimensions are constantly shrinking, understanding the physical properties emerging at interfaces is crucial to exploit them for applications. Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. We combine the features of both materials by investigating from first principles and Monte Carlo simulations the interface between graphene and $BaMnO_3$, a magneto-electric multiferroic. We show [1] that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. A remarkably large proximity induced spin splitting of the Dirac cones ($\approx$ 300 meV) is achieved and doping can make the high-mobility region of the electronic bands experimentally accessible.

Spin-Orbit Coupling calculations reveal that graphene deeply affects the magnetic state of the substrate, down to several layers below the interface, by inducing an overall magnetic softening, and switching the in-plane magnetic ordering from anti- to ferromagnetic. The graphene-BaMnO3 system presents a SOC gap 300 times larger than in pristine graphene, leading to a new flavor of Quantum Anomalous Hall effect (QAHE), a hybrid QAHE, characterized by the coexistence of metallic and topological insulating states. These findings could be exploited to fabricate novel devices that use graphene to control the magnetic configuration of a substrate [2].

Funding: Ramon y Cajal RYC-2016-19344 (MINECO/AEI/FSE, UE), H2020-INFRAEDI-2018-2020 MaX CoE (grant nr. 824143), PGC2018-096955-B-C43 (MICIU/AEI/FEDER, UE) ICN2 is supported by the Severo Ochoa Centres of Excellence programme, funded by the Spanish Research Agency (AEI grant No. SEV-2017-0706) and by the CERCA programme of the Generalitat de Catalunya (2017SGR1506)

Computing time: RES on MareNostrum (Barcelona Supercomputing Center), PRACE-3IP and 4IP on Lindgren, Archer, and Salomon (EU Grants No. RI-312763 and No. 653838), JARA-HPC (No. jara0088, No. JIAS16, and No. JHPC39)

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Coupled spin-lattice dynamics with multibinit

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Density functional theory (DFT) has become the workhorse in simulating materials properties, thanks to a better system size scaling ($O(N^3)$) than full many-body methods. However, to simulate the dynamics of large systems, especially with coupled degrees of freedom, it reaches its limits. In order to overcome these limits without completely losing the ab initio predictive power, we construct a model Hamiltonian with parameters determined from DFT calculations, which we then use to simulate dynamical processes with up to tens of thousands of atoms. We have implemented the method for lattice-, spin-, and coupled spin-lattice systems in the multibinit code. The code uses an abstract layer for the different potential energy terms, which allows for an easy inclusion of further terms in the model Hamiltonian in the future. As expected, the complexity is in fitting a good set of parameters. As we did not expect, even the choice of the model Hamiltonian and the coupling terms is non-trivial. We show results for a simple magnetic perovskite SrMnO3, which is known to host a very large spin phonon coupling.

Understanding 2D magnetic junctions from fabrication to new functionalities

Simon Dubois

Unité mixte de Physique CNRS/Thales (France) and
UCLouvain, Nanoscopic Physics Group (Belgium)

Two-dimensional materials are promising candidates for use as tunnel barrier in atomically thin magnetic tunnel junctions (MTJs). High magneto resistance ratios have been predicted theoretically and recent progress in large scale manufacturing of these materials has paved the way towards their integrations in functional devices. Yet, the experimental results available so far vary greatly depending on the integration pathways. Here, we show that first-principles calculations can provide useful insights into the close relation that links the interface morphology to its magneto resistive behaviour. In particular, we illustrate the phenomena of hybridization, charge transfert and momentum selection in based 2D-MTJs based on h-BN, graphene and TMDCs .

Spin States Protected from Intrinsic Electron-Phonon Coupling in $MoSe_2$

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Measurements in monolayer $MoSe_2$ of the Kerr rotation have show spin lifetimes of over 100 ns at room temperature. These are also accompanied by a non monotone temperature dependence of the Kerr amplitude, which increases with temperature up to 50 K, having then an abrupt sign change. With ab initio simulations we can explain the latter behaviour as an effect of the intrinsic electron-phonon coupling and possibility of electrons to transit into secondary valleys. The electron-phonon scattering mechanism begins this scattering process within the first picoseconds after excitation. The sign of the resulting magnetisation, and so the Kerr amplitude as well, changes signal as a function of temperature, as electrons and holes have different changes in intervalley scattering rates. Our ab initio calculations do not, however, provide a reason for the long spin lifetimes. This leads us to the conclusion that the some of the initial spin polarisation must be stored into spin states which are protected from the intrinsic electron-phonon interaction. These states are most likely resident charge carriers, which are not part of the itinerant valence or conduction band states.

Thermal and electronic transport characteristics of highly stretchable graphene kirigami

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For centuries, cutting and folding papers with special patterns have been used to build beautiful, flexible and complex three-dimensional structures. Inspired by the old idea of kirigami (paper cutting), and the outstanding properties of graphene, recently graphene kirigami structures were fabricated to enhance the stretchability of graphene. However, the possibility of further tuning the electronic and thermal transport along the 2D kirigami structures has remained original to investigate. We therefore performed extensive atomistic simulations to explore the electronic, heat and load transfer along various graphene kirigami structures. The mechanical response and thermal transport were explored using classical molecular dynamics simulations. We then used a real-space Kubo–Greenwood formalism to investigate the charge transport characteristics in graphene kirigami. Our results reveal that graphene kirigami structures present highly anisotropic thermal and electrical transport. Interestingly, we show the possibility of tuning the thermal conductivity of graphene by four orders of magnitude. Moreover, we discuss the engineering of kirigami patterns to further enhance their stretchability by more than 10 times as compared with pristine graphene. Our study not only provides a general understanding concerning the engineering of electronic, thermal and mechanical response of graphene, but more importantly can also be useful to guide future studies with respect to the synthesis of other 2D material kirigami structures, to reach highly flexible and stretchable nanostructures with finely tunable electronic and thermal properties.

Origin and mechanism of the metal-insulator transition in perovskite nickelates, manganites and ferrites.

Philippe Ghosez

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ABO_3 perovskite oxides, with a transition metal at the B site, form a broad family of compounds, which are fascinating by the diversity of their functional properties. Among them, different series of perovskites with formal e_g^1 occupation of the d-orbitals at the B site, such as rare-earth manganites ($RMnO_3$), rare-earth nickelates ($RNiO_3$) or alkaline-earth ferrites ($AFeO_3$), are similarly prone to show a metal-insulator transition (MIT). However, the mechanism behind such a transition can be intriguingly different from one series to the other, being for instance related to electronic charge ordering and atomic breathing distortion in nickelates and to electronic orbital ordering and atomic Jahn-Teller distortion in manganites.

Focusing first on rare-earth nickelates, it will be shown that the charge-ordered MIT in this series can be seen as a structurally triggered phase transition [1], highlighting a first concrete example of such a kind of phase transition in simple perovskites. The origin of this unusual mechanism will be traced back in the electronic and magnetic properties of nickelates, revealing a Peierls-type instability, structurally triggered by oxygen rotation motions and eventually assisted by magnetic ordering. This knowledge will be used to rationalize the evolution of the MIT in thin films and heterostructures [2]. The discussion will then be extended to alkaline-earth ferrites [3] and rare-earth manganites [4], highlighting that electronic charge and orbital orderings typically com-pete in eg1 perovskites to produce the MIT and are both strongly coupled to lattice degrees of freedom. The behavior of the different series will be discussed, revealing also how to eventually switch from one type of ordering to the other using strain engineering.

Work done in collaboration with Alain Mercy, Yajun Zhang, Marcus Schmitt, He Xu, Jordan Bied-er & Eric Bousquet. Research supported by ARC project AIMED and ERA.NET project SIOX.

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Two-dimensional orbital Hall insulators

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The field of spintronics blossomed in the last decade, as a consequence of the use of spin-orbit coupling to generate and manipulate spin currents in non-magnetic materials. In these systems, the efficient conversion between charge and spin currents is mediated by spin-orbit. Great progress in the manipulation of the orbital angular momentum of light has also been achieved in the last decades, leading to a large number of relevant applications. Still, electron orbitals in solids were less exploited, even though they are known to be essential in several underlying physical processes in material science. The orbital-Hall effect (OHE), similarly to the spin-Hall effect (SHE), refers to the creation of a transverse flow of orbital angular momentum that is induced by a longitudinally applied electric field. The OHE has been explored mostly in metallic systems, where it can be quite strong. However, several of its features remain unexplored in two-dimensional (2D) materials.

We then investigate the OHE in multi-orbital 2D insulators, such as transition metal dichalcogenides. We show that the OHE in these systems is associated with exotic momentum-space orbital textures. This intrinsic property emerges from the interplay between orbital attributes and crystalline symmetries and does not rely on the spin-orbit coupling. Our results indicate that multi-orbital 2D materials can display robust OHE that may be used to generate orbital angular momentum accumulation, and produce strong orbital torques that are of great interest for developing novel spin-orbitronic devices.

Theoretical Spectroscopy of 2D Materials: Exciton-phonon coupling in resonant Raman and luminescence spectroscopy

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2D materials are known to exhibit very pronounced excitonic effects due to the confinement of electrons and holes in a layer and due to the weak dielectric screening of the electron-hole interaction. In spectroscopy involving vibrational degrees of freedom, the exciton-phonon coupling must therefore be included in order to obtain a qualitative understanding of the spectra and in order to obtain quantitative results. We present our methods for the calculation of exciton-phonon coupling via a finite displacement and via a diagrammatic approach, both using many-body perturbation theory.

We present results for the phonon-assisted luminescence spectrum of bulk hexagonal boron nitride (hBN), where the combination of indirect band gap and strong excitonic effects leads to a complex peak structure due to coupling of excitons with various phonon branches. Furthermore, we present calculations of resonant Raman intensities with the combined inclusion of both excitonic and non-adiabatic effects. In bulk hBN, which has high phonon-frequencies due to the light atoms, we demonstrate the emergence of strong quantum interference between different excitonic resonances due to non-adiabatic effects. In MoS_2 and $MoTe_2$, our calculations explain the observed different intensity dependences of the A1' and E' modes on the exciting laser frequency.

Plasmons in nanostructured and corrugated 2D materials

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Plasmons are extensively investigated due to their capacity to concentrate electromagnetic energy to scale smaller than the wavelength and because they govern the optical response of nanomaterials. The 1D plasmons at the edge of 2D finite domains or at the interfaces between conducting and insulating 2D materials have been suggested as the analog of the 2D surface or interface plasmons well known in metallic films. Another type of 1D plasmons is associated to atomic reconstructions at the edge of nanoribbon or at grain boundaries that can be at the origin of a 1D metallic channel in 2D materials. In this work, we theoretically examine metallic behavior of experimentally observed mirror twin boundaries in transition metal dichalcogenide (TMDs). We also investigate the optical response of corrugated graphene films. We evidence the appearance of plasmon excitation in the IR/Visible related to the corrugation and compare them with recent SERS experimental data. The plasmonic excitations are analyzed using an eigenmode decomposition of the microscopic dielectric function obtained by DFT simulations available in the GPAW code. We link these ab initio results with classical approach and effective medium theory approach. Acknowledgements Computational

Graphene plasmonics: exploring the nonlocal response of 2D electron liquids

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Plasmons, being collective density oscillations of the electronic liquid are sensitive to both the surroundings of the material in which they occur, and to the intrinsic properties of the electronic liquid in which they appear [1]. Because plasmons represent wave-like excitations of the electron liquid, they directly depend on the nonlocal and dynamical properties of that liquid. Therefore, the study of propagating plasmons can yield insight in these properties, which are often difficult to access experimentally. With the onset of two-dimensional materials, it became, furthermore, possible to tune the material's environment and intrinsic properties like the electron density, allowing us to directly measure some of the parameters that determine the Fermi liquid properties of these 2D electron liquids.

In this talk, I will explain how quantum nonlocal properties of the electron liquid of graphene can be inferred by tuning the dielectric environment and investigating the plasmonic dispersion relation and plasmon velocity [2]. Further, I show how one can tune the dynamics of these plasmons to investigate the crossover between collisionless and the newly found hydrodynamic regimes [3] of a 2D electronic liquid and how the plasmon group velocity and damping acts as hallmarks of the different regimes [4].

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Perfect electromagnetic absorbers: a road to reality

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We use a genetic algorithm to optimize 2-D periodic arrays of truncated square-based pyramids made of only one, two or three stacks of metal/dielectric layers. The objective is to achieve a quasi-perfect broadband absorption of normally incident radiations with wavelengths comprised between 420 and 1600 nm. Previous work by Lobet et al. [1] has shown that ultra-broadband absorption can be achieved with periodic arrays of truncated square-based pyramids made of alternating metal/dielectric layers. By using 20 stacks of Au/Ge layers, they could indeed absorb 98% of incident radiations with wavelengths between 0.2 and 5.8 microns. This ultra-broadband absorption is essentially due to (i) an efficient anti-reflection property of these pyramidal structures and (ii) a well-designed coupling between the localized surface plasmons found at the metal/dielectric interfaces of each stack. Since the fabrication of structures made of 20 stacks of metal/dielectric layers is not practical, we use a genetic algorithm to establish simplified structures that consist of only 1, 2 or 3 stacks of metal/dielectric layers. We consider in particular the results one can obtain by considering (i) Ni, Ti, Al or Cr for the metal, and (ii) poly(methyl methacrylate) (PMMA) or TiO_2 for the dielectric. The parameters to determine for each metal/dielectric combination are (i) the period of the system, (ii) the lateral dimensions of each stack of metal/dielectric layers and (iii) the width of each dielectric layer. These parameters are subject to the constraint that the final structure must form a realistic pyramidal structure. The increased number of degrees of freedom in the structures considered is expected to compensate the reduced number of metal/dielectric layers. We use a Rigorous Coupled Waves Analysis (RCWA) method to compute the absorption spectrum of the structures considered. A parallel version of the genetic algorithm [2,3] is then used to solve the optimization problem and establish high-quality solutions. Our study shows that Ni/PMMA represents the best metal/dielectric combination. With an optimized structure made of only three stacks of Ni/PMMA, it is possible indeed to absorb 99.8% of the considered incident radiations. An integrated absorptance of 99.4% is achieved with three stacks of Ti/PMMA or Cr/PMMA layers. Aluminium is not to recommend for this application. As shown by the maps established by the genetic algorithm, the solutions obtained with Aluminium are indeed too sensitive on the geometrical parameters of the system.

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MXenes: the largest family of 2D materials

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Two-dimensional (2D) materials have attracted huge attention in nanotechnology thanks to the enhanced low-dimensional quantum effects, resulting in outstanding electronic, optical, and magnetic properties. Among these 2D systems, the emerging family of 2D transition metal carbides and nitrides, known as MXenes, stands out because of the wide chemical diversity allowing for materials property tuning. In contrast to graphite-like layered materials which can be mechanically exfoliated to obtain 2D flakes, MXenes are obtained from the chemical treatment of the three-dimensional MAX phases. MAX phases are layered ceramics with the general formula $M_{n+1}AX_n$, where M represents an early transition metal, A an element from groups 13 to 16, X either a carbon or a nitrogen atom, and n varies from 1 to 3. Since the discovery of the first MXene, Ti_3C_2, at Drexel University in 2011, more than 30 MXenes have been synthesized, and the stability and properties of dozens more have been investigated using ab initio calculations.

The exploration of new MAX phases and derivative MXenes is of great interest to further control materials properties and highlight potential applications, such as catalysis, energy storage and related electrochemical applications.

In this talk, the different classes of MAX phases and their 2D counterparts, MXenes, will be introduced and their respective structural, electronic, and elastic properties predicted by ab initio calculations and characterized by various experimental techniques will be discussed.

Electron-phonon Scattering in 2D materials: a quest for high conductivity

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Recently, some of us identified close to 2000 exfoliable 2D materials from first-principles calculations [1]. We are now characterizing the scattering of electrons by phonons in this database, with the objective of finding elewctrostatically-doped 2D semiconductors with superior intrinsic transport properties. We use an approximate descriptor to scan hundreds of materials in the database and find outstanding candidates. We then use a high-accuracy method [2] to compute the conductivity of selected materials (50). Several novel high-conductivity 2D materials are found and the data provides valuable insights on electron-phonon scattering. Three aspects stand out: intervalley scattering, doping, and band anisotropy. We will briefly discuss their impact on transport, and how they can be exploited to find or engineer 2D semiconductors with high conductivities.

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Understanding phonons in slightly-misaligned graphene bilayer with the Frenkel-Kontorova model

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The discovery of unconventional superconductivity in graphene bilayer twisted by a 1.08° twist angle [1] has triggered a renewed interest from the scientific community for the system. While many efforts have already been provided to understand its electronic properties [2], surprinsingly little has yet been done to characterize its phonon spectrum.

In this work, we investigate the phonons in twisted graphene bilayers using force fields. The emergence of phonon side bands at the zone center and at the zone borders of graphene is highlighted, especially for small mislignement angles between the layers. Those side bands are explained using the Frenkel-Kontorova model [2] and are found to directly arise from the formation of a soliton network in the system. We discuss how the problem can actually be seen as the counterpart for phonons of the Nearly-Free Electron model [3], where the electrons and the nucleus potential have been replaced by the phonons and the soliton potential, respectively.

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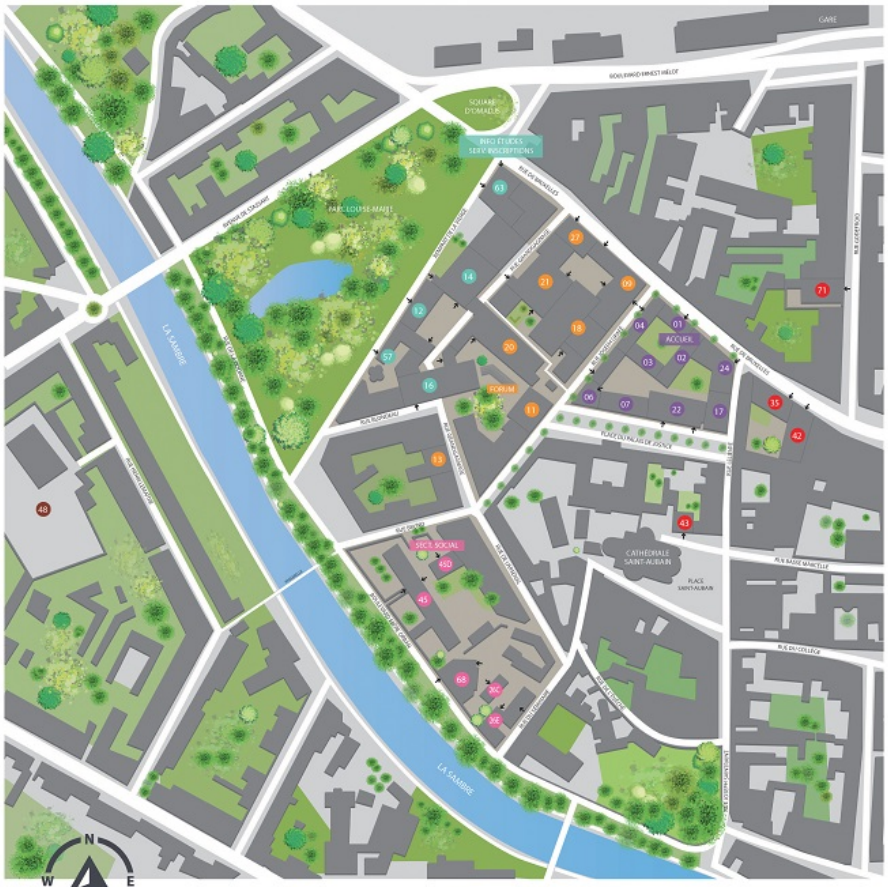

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